



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 PM UTC

PDB ID : 3PCN / pdb_00003pcn
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3,4-DIHYDROXYPHENYLACETATE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-08-19
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

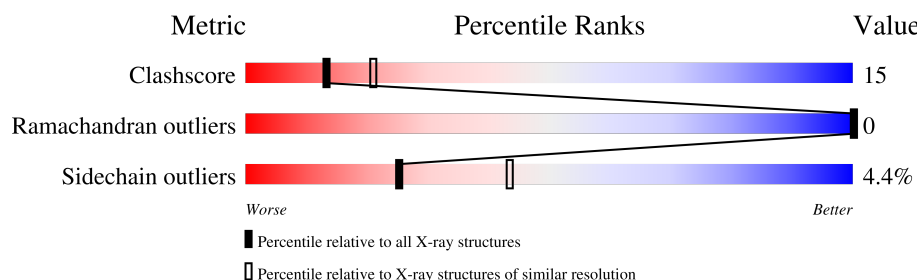
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	72% 25% .
1	B	200	72% 25% .
1	C	200	68% 26% 5% .
1	D	200	72% 26% .
1	E	200	68% 28% .
1	F	200	69% 26% 5%
2	M	238	67% 26% . .
2	N	238	72% 21% . .

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Mol	Chain	Length	Quality of chain
2	O	238	 71%25% . .
2	P	238	 71%23% . .
2	Q	238	 67%25%5% .
2	R	238	 63%30% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DHY	Q	550[A]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

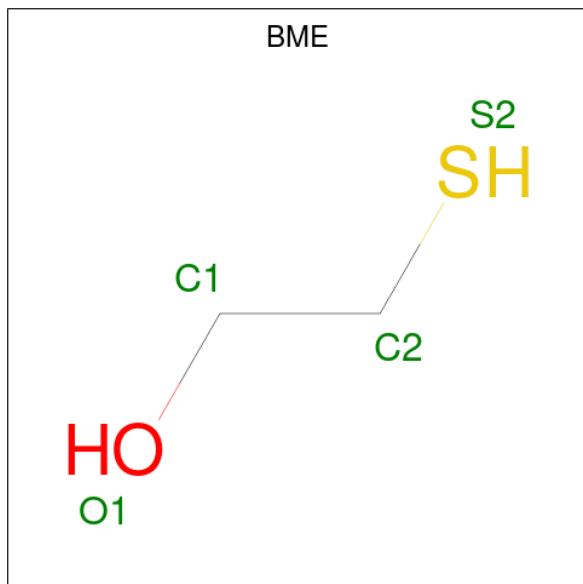
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	N	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	O	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	P	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	R	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

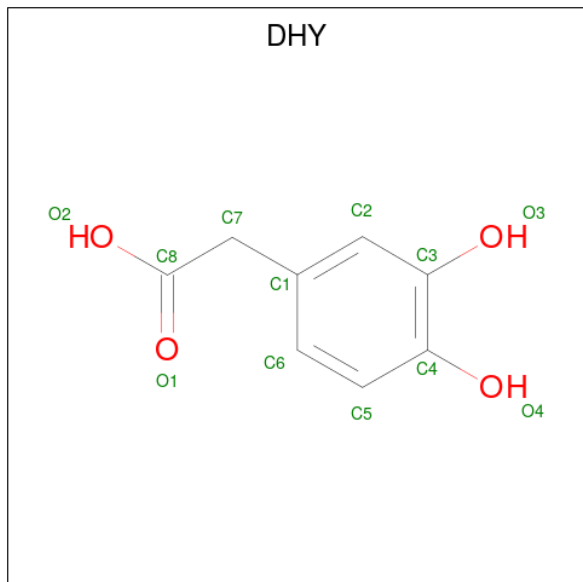
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 2-(3,4-DIHYDROXYPHENYL)ACETIC ACID (CCD ID: DHY) (formula: $C_8H_8O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	1
			24	16	8		
5	N	1	Total	C	O	0	1
			24	16	8		
5	O	1	Total	C	O	0	1
			24	16	8		
5	P	1	Total	C	O	0	1
			24	16	8		
5	Q	1	Total	C	O	0	1
			24	16	8		
5	R	1	Total	C	O	0	1
			24	16	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	M	150	Total	O	0	0
			150	150		
6	B	79	Total	O	0	0
			79	79		
6	N	152	Total	O	0	0
			152	152		

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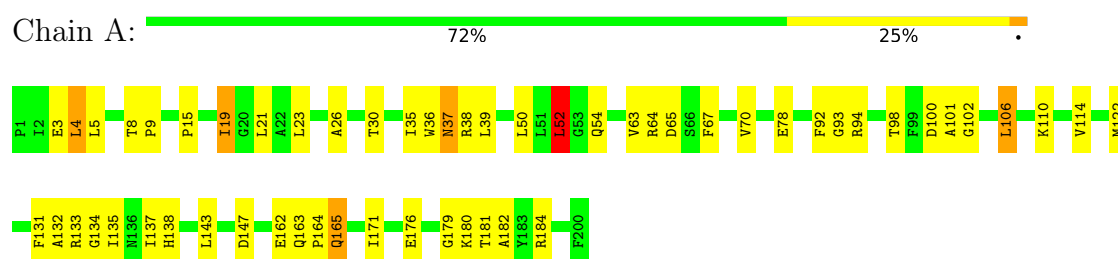
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	81	Total 81	O 81	0	0
6	O	147	Total 147	O 147	0	0
6	D	82	Total 82	O 82	0	0
6	P	145	Total 145	O 145	0	0
6	E	80	Total 80	O 80	0	0
6	Q	149	Total 149	O 149	0	0
6	F	79	Total 79	O 79	0	0
6	R	150	Total 150	O 150	0	0

3 Residue-property plots

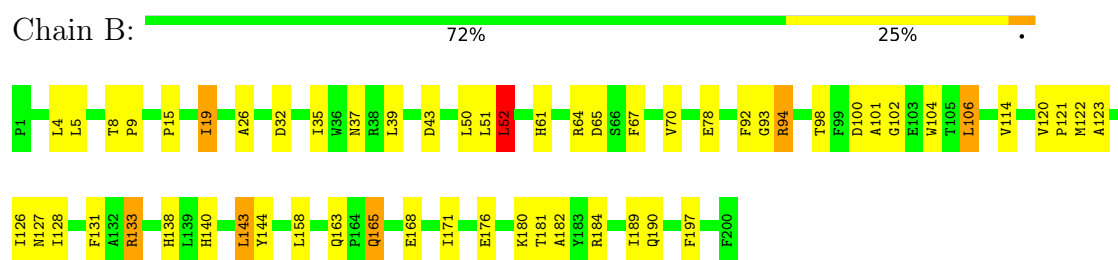
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

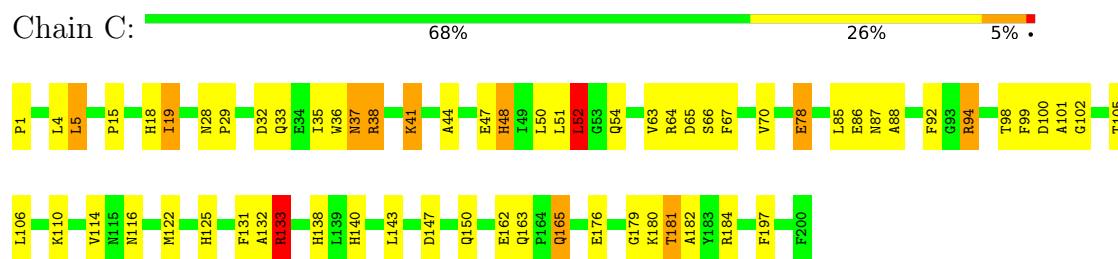
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



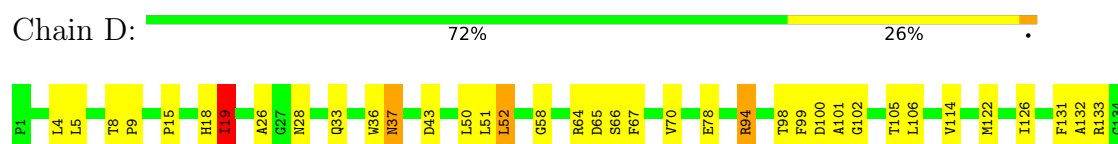
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



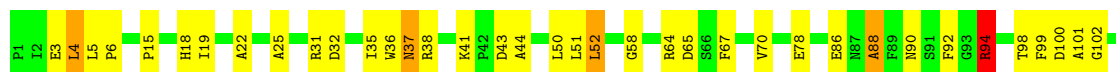
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





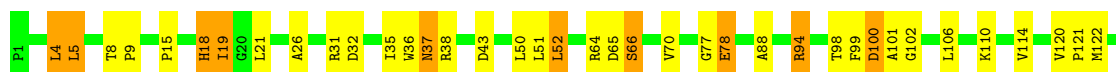
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 68% 28% .



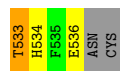
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 69% 26% 5%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 67% 26% . .



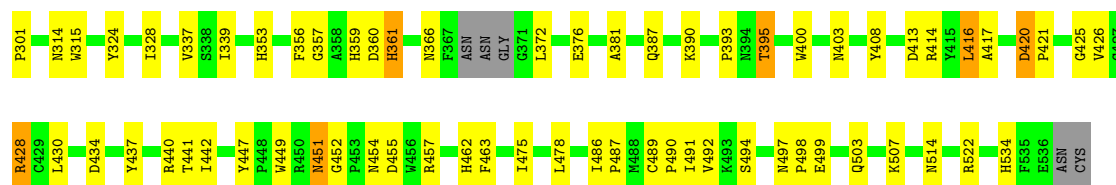
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N: 72% 21% . .



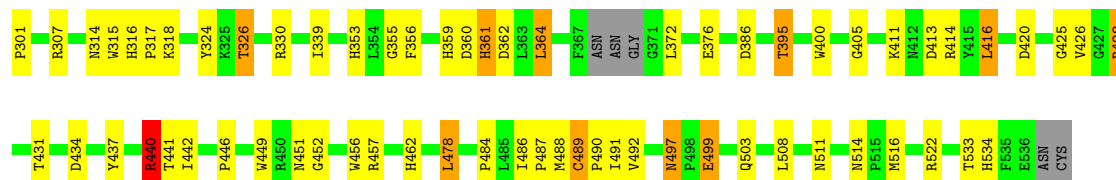
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O: 71% 25% . .



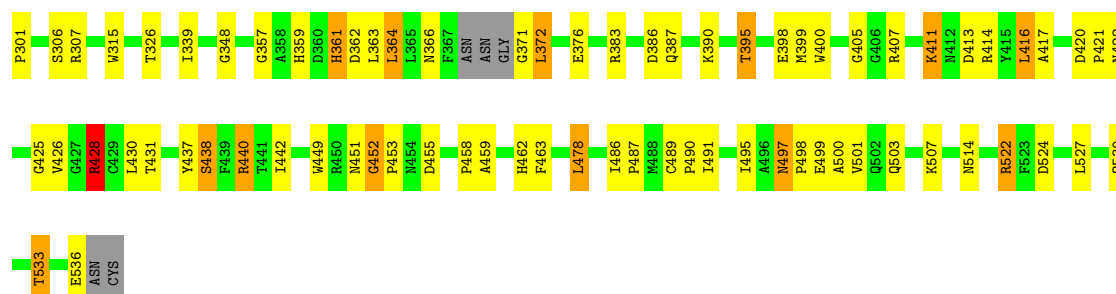
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



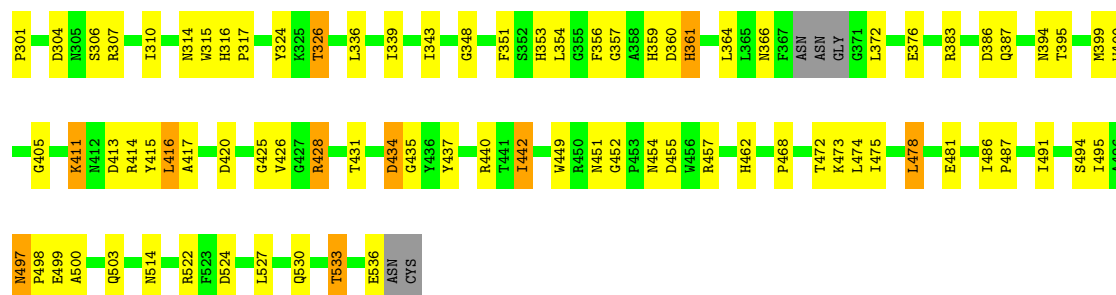
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.60 Å 127.50 Å 134.30 Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.0 (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22014	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, DHY, BME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	0/1611	1.63	10/2195 (0.5%)
1	B	1.05	1/1611 (0.1%)	1.61	8/2195 (0.4%)
1	C	1.05	0/1611	1.59	15/2195 (0.7%)
1	D	1.02	0/1611	1.54	8/2195 (0.4%)
1	E	1.07	1/1611 (0.1%)	1.61	16/2195 (0.7%)
1	F	1.13	2/1611 (0.1%)	1.75	15/2195 (0.7%)
2	M	1.10	0/1895	1.66	17/2580 (0.7%)
2	N	1.08	1/1895 (0.1%)	1.63	13/2580 (0.5%)
2	O	1.11	2/1895 (0.1%)	1.69	26/2580 (1.0%)
2	P	1.11	2/1895 (0.1%)	1.66	18/2580 (0.7%)
2	Q	1.15	1/1895 (0.1%)	1.61	21/2580 (0.8%)
2	R	1.15	0/1895	1.66	26/2580 (1.0%)
All	All	1.09	10/21036 (0.0%)	1.64	193/28650 (0.7%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	451	ASN	CA-C	7.46	1.55	1.52
1	B	94	ARG	CD-NE	-6.40	1.37	1.46
2	N	441	THR	CA-CB	6.31	1.61	1.54
1	F	94	ARG	NE-CZ	-5.83	1.26	1.33
1	F	94	ARG	CD-NE	-5.76	1.38	1.46
2	O	441	THR	CA-CB	5.71	1.61	1.53
2	O	451	ASN	CA-C	5.57	1.55	1.52
1	E	108	THR	CA-CB	5.33	1.61	1.54
2	Q	452	GLY	N-CA	5.30	1.51	1.44
2	P	441	THR	CA-CB	5.14	1.60	1.53

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	94	ARG	CD-NE-CZ	25.81	160.53	124.40
1	F	94	ARG	CA-CB-CG	17.55	149.19	114.10
2	Q	452	GLY	N-CA-C	-10.69	99.29	112.23
2	O	452	GLY	N-CA-C	-10.54	99.48	112.23
2	N	452	GLY	N-CA-C	-10.14	99.63	112.10
2	R	361	HIS	CA-CB-CG	-9.82	103.98	113.80
1	D	37	ASN	N-CA-C	9.60	123.68	112.93
2	O	451	ASN	O-C-N	9.59	127.92	120.83
2	P	452	GLY	N-CA-C	-9.39	100.87	112.23
2	M	339	ILE	O-C-N	9.12	127.44	121.69
2	P	451	ASN	O-C-N	9.03	127.51	120.83
2	O	353	HIS	CA-CB-CG	-8.23	105.57	113.80
1	B	94	ARG	CG-CD-NE	8.22	130.09	112.00
1	B	94	ARG	CD-NE-CZ	8.16	135.82	124.40
1	F	43	ASP	CA-CB-CG	-8.09	104.51	112.60
1	E	99	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	37	ASN	N-CA-C	7.89	121.77	112.93
2	P	361	HIS	CA-CB-CG	-7.87	105.93	113.80
1	F	38	ARG	CA-CB-CG	7.64	129.39	114.10
1	B	37	ASN	N-CA-C	7.61	122.15	113.02
1	D	19	ILE	CB-CA-C	7.58	122.37	112.14
1	E	37	ASN	N-CA-C	7.58	121.92	113.21
1	C	37	ASN	N-CA-C	7.51	121.34	112.93
2	Q	428	ARG	CD-NE-CZ	7.45	134.83	124.40
1	E	90	ASN	CA-CB-CG	7.28	119.88	112.60
1	F	37	ASN	N-CA-C	7.19	120.98	112.93
2	Q	361	HIS	CA-CB-CG	-7.15	106.65	113.80
2	Q	339	ILE	O-C-N	7.15	126.19	121.69
2	R	353	HIS	CA-CB-CG	-7.15	106.65	113.80
2	N	361	HIS	CA-CB-CG	-7.05	106.75	113.80
1	F	94	ARG	CB-CG-CD	6.87	127.11	111.30
1	E	94	ARG	CA-CB-CG	6.80	127.71	114.10
2	Q	372	LEU	N-CA-C	-6.74	100.14	110.32
2	Q	440	ARG	NE-CZ-NH2	-6.73	113.14	119.20
2	Q	514	ASN	O-C-N	6.61	127.41	121.19
1	C	87	ASN	CA-CB-CG	6.57	119.17	112.60
2	M	494	SER	N-CA-C	-6.56	104.37	112.38
2	M	353	HIS	CA-CB-CG	-6.53	107.27	113.80
1	E	38	ARG	CD-NE-CZ	-6.47	115.34	124.40
1	A	3	GLU	CB-CG-CD	6.46	123.59	112.60
1	E	5	LEU	N-CA-C	-6.45	101.63	109.83
1	E	88	ALA	N-CA-C	-6.44	104.90	112.89
2	R	475	ILE	N-CA-CB	6.42	120.26	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	337	VAL	CA-C-O	-6.35	113.67	120.59
1	F	5	LEU	O-C-N	6.34	128.53	121.43
1	A	5	LEU	N-CA-C	-6.34	101.78	109.83
2	O	372	LEU	N-CA-C	-6.34	100.75	110.32
2	P	372	LEU	CB-CA-C	6.31	117.45	108.68
2	R	420	ASP	CB-CA-C	6.26	117.11	110.17
2	N	434	ASP	CA-CB-CG	-6.25	106.35	112.60
2	M	457	ARG	CD-NE-CZ	6.22	133.11	124.40
1	C	52	LEU	CB-CA-C	6.20	123.79	110.45
1	B	133	ARG	CA-CB-CG	6.20	126.50	114.10
2	O	463	PHE	CA-CB-CG	6.18	119.98	113.80
2	R	440	ARG	CD-NE-CZ	-6.17	115.77	124.40
2	N	440	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	F	5	LEU	N-CA-C	-6.16	102.01	109.83
1	A	23	LEU	CB-CA-C	6.04	120.77	110.74
2	N	533	THR	CA-CB-OG1	-6.03	100.55	109.60
2	O	361	HIS	CA-CB-CG	-6.01	107.79	113.80
2	R	411	LYS	CB-CA-C	-6.01	100.87	110.84
2	R	336	LEU	CA-C-O	-5.97	115.05	121.56
2	P	386	ASP	CB-CA-C	5.97	120.77	110.45
2	M	326	THR	CA-CB-OG1	-5.97	100.65	109.60
2	N	494	SER	N-CA-C	-5.93	105.14	112.38
2	R	494	SER	N-CA-C	-5.92	105.31	112.54
2	O	339	ILE	O-C-N	5.91	125.42	121.69
2	O	434	ASP	CA-CB-CG	-5.91	106.69	112.60
2	O	440	ARG	NE-CZ-NH2	-5.90	113.89	119.20
2	O	440	ARG	CD-NE-CZ	-5.90	116.14	124.40
2	N	440	ARG	CD-NE-CZ	-5.89	116.16	124.40
2	R	357	GLY	N-CA-C	-5.88	105.01	112.54
2	O	314	ASN	CB-CA-C	5.85	119.83	109.65
2	R	434	ASP	CA-CB-CG	-5.85	106.75	112.60
1	D	52	LEU	CB-CA-C	5.85	122.39	109.94
1	F	88	ALA	N-CA-C	-5.83	106.00	113.23
2	Q	411	LYS	CB-CA-C	-5.83	101.17	110.84
2	R	454	ASN	CA-CB-CG	5.83	118.43	112.60
2	R	481	GLU	CB-CG-CD	5.82	122.50	112.60
2	O	372	LEU	CB-CA-C	5.82	116.73	108.76
1	E	171	ILE	N-CA-CB	-5.81	104.41	111.21
2	R	533	THR	N-CA-C	-5.81	102.86	110.53
2	N	514	ASN	O-C-N	5.79	126.70	120.85
2	R	339	ILE	O-C-N	5.79	125.34	121.69
2	P	339	ILE	O-C-N	5.78	125.33	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	GLU	CB-CG-CD	5.77	122.41	112.60
2	P	489	CYS	N-CA-C	5.76	117.94	109.42
2	M	306	SER	N-CA-C	5.73	118.95	110.46
2	R	326	THR	CA-CB-OG1	-5.73	101.00	109.60
1	C	38	ARG	CD-NE-CZ	-5.73	116.38	124.40
2	M	361	HIS	CA-CB-CG	-5.70	108.10	113.80
2	P	353	HIS	CA-CB-CG	-5.70	108.11	113.80
1	C	125	HIS	CA-CB-CG	-5.68	108.12	113.80
2	P	457	ARG	CA-CB-CG	5.64	125.39	114.10
2	O	420	ASP	CB-CA-C	5.64	116.43	110.17
2	Q	522	ARG	CD-NE-CZ	-5.63	116.52	124.40
2	M	372	LEU	N-CA-C	-5.62	102.55	110.31
2	N	354	LEU	CB-CA-C	5.61	119.25	109.65
2	M	454	ASN	CA-CB-CG	5.60	118.20	112.60
2	O	494	SER	N-CA-C	-5.59	105.56	112.38
1	E	171	ILE	CB-CA-C	5.59	118.64	110.98
2	Q	497	ASN	CB-CA-C	5.58	117.41	109.38
1	C	47	GLU	CB-CG-CD	5.57	122.08	112.60
2	P	440	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	C	150	GLN	N-CA-CB	5.56	118.07	110.01
2	R	314	ASN	N-CA-C	-5.53	106.70	113.50
1	F	141	THR	CA-CB-CG2	5.52	119.88	110.50
1	D	28	ASN	O-C-N	5.50	126.03	121.35
2	M	533	THR	N-CA-C	-5.50	102.75	110.50
1	D	137	ILE	CB-CA-C	5.50	118.36	110.33
1	E	18	HIS	CA-CB-CG	-5.49	108.31	113.80
2	P	314	ASN	N-CA-C	-5.49	106.75	113.50
2	O	492	VAL	N-CA-C	-5.48	105.03	110.62
2	P	359	HIS	CA-CB-CG	-5.48	108.32	113.80
1	F	189	ILE	O-C-N	5.48	127.47	121.83
2	R	394	ASN	CA-CB-CG	-5.48	107.12	112.60
2	M	460	HIS	CA-CB-CG	-5.47	108.33	113.80
2	R	452	GLY	N-CA-C	-5.47	101.17	112.34
1	C	99	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	189	ILE	O-C-N	5.45	127.16	121.87
2	O	514	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	21	LEU	N-CA-C	5.44	120.79	113.72
1	E	43	ASP	CA-CB-CG	-5.40	107.20	112.60
2	M	457	ARG	CA-CB-CG	5.38	124.85	114.10
1	D	94	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	F	21	LEU	N-CA-CB	-5.37	103.47	110.88
1	C	5	LEU	N-CA-C	-5.37	103.01	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	LEU	CB-CA-C	5.36	121.98	110.45
2	O	417	ALA	N-CA-C	-5.35	103.04	109.83
1	E	189	ILE	O-C-N	5.34	127.05	121.87
2	O	339	ILE	CB-CA-C	5.34	114.56	109.33
2	M	417	ALA	N-CA-C	-5.33	103.06	109.83
2	O	475	ILE	N-CA-CB	5.33	118.77	111.41
2	N	452	GLY	CA-C-O	-5.32	117.30	122.46
2	R	514	ASN	CB-CA-C	5.32	115.44	110.17
2	M	452	GLY	N-CA-C	-5.31	101.52	112.34
1	C	133	ARG	CA-CB-CG	5.30	124.71	114.10
1	F	18	HIS	CA-CB-CG	-5.30	108.50	113.80
1	E	125	HIS	CA-CB-CG	-5.29	108.51	113.80
1	C	41	LYS	N-CA-C	-5.29	102.52	110.24
2	M	503	GLN	OE1-CD-NE2	5.28	127.88	122.60
2	P	514	ASN	CB-CA-C	5.28	116.04	110.17
1	D	43	ASP	CA-CB-CG	-5.28	107.32	112.60
1	F	165	GLN	CB-CG-CD	5.27	121.55	112.60
1	B	5	LEU	N-CA-C	-5.26	103.15	109.83
2	N	475	ILE	N-CA-CB	5.26	118.66	111.41
1	B	52	LEU	CB-CA-C	5.25	121.12	109.94
2	R	514	ASN	O-C-N	5.24	126.12	121.19
2	Q	514	ASN	CA-CB-CG	5.24	117.84	112.60
1	C	5	LEU	O-C-N	5.24	127.30	121.43
2	O	457	ARG	CA-CB-CG	5.23	124.56	114.10
2	Q	348	GLY	O-C-N	5.23	127.00	121.77
2	N	514	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	30	THR	CA-CB-OG1	-5.20	101.80	109.60
2	O	454	ASN	CA-CB-CG	5.20	117.80	112.60
2	Q	459	ALA	N-CA-C	-5.19	102.36	110.10
2	P	441	THR	N-CA-CB	-5.19	102.87	110.97
2	O	440	ARG	NH1-CZ-NH2	5.19	126.04	119.30
1	C	18	HIS	CA-CB-CG	-5.18	108.62	113.80
1	F	100	ASP	CA-CB-CG	-5.18	107.42	112.60
2	O	428	ARG	CD-NE-CZ	5.17	131.64	124.40
1	A	137	ILE	CB-CA-C	5.17	117.87	110.33
1	C	48	HIS	CA-CB-CG	-5.17	108.63	113.80
1	E	171	ILE	N-CA-C	5.16	115.52	107.99
2	Q	501	VAL	O-C-N	5.16	126.87	121.87
2	R	457	ARG	CA-CB-CG	5.14	124.39	114.10
2	P	372	LEU	N-CA-C	-5.13	103.22	110.31
2	O	357	GLY	N-CA-C	-5.13	105.98	112.54
1	A	21	LEU	N-CA-CB	-5.12	103.12	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	316	HIS	O-C-N	5.10	127.00	121.60
1	E	52	LEU	CB-CA-C	5.09	121.40	110.45
2	R	324	TYR	CA-C-N	5.09	128.46	120.82
2	R	324	TYR	C-N-CA	5.09	128.46	120.82
2	Q	463	PHE	O-C-N	5.07	129.48	123.24
2	N	367	PHE	CA-C-O	-5.07	112.18	120.80
2	P	420	ASP	CB-CA-C	5.07	115.98	110.15
1	D	5	LEU	O-C-N	5.07	126.34	121.28
2	Q	533	THR	CA-CB-OG1	-5.06	102.00	109.60
1	C	32	ASP	O-C-N	5.06	127.35	122.09
2	M	386	ASP	CA-CB-CG	5.05	117.66	112.60
2	P	395	THR	CA-CB-OG1	-5.05	102.02	109.60
2	Q	458	PRO	N-CA-C	-5.05	103.84	111.41
1	A	171	ILE	N-CA-C	5.05	115.03	107.51
2	O	447	TYR	O-C-N	5.04	126.22	121.38
2	Q	357	GLY	N-CA-C	-5.04	106.09	112.54
2	P	326	THR	CA-CB-OG1	-5.04	102.04	109.60
2	R	457	ARG	CD-NE-CZ	5.04	131.45	124.40
2	Q	438	SER	O-C-N	5.03	129.05	123.52
2	R	354	LEU	CB-CA-C	5.02	118.24	109.65
2	Q	438	SER	N-CA-CB	5.02	119.10	110.77
2	Q	428	ARG	NE-CZ-NH2	-5.01	114.69	119.20
2	R	348	GLY	O-C-N	5.01	126.78	121.77
1	B	43	ASP	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	48	0
1	B	1571	0	1499	46	0
1	C	1571	0	1499	52	0
1	D	1571	0	1499	47	0
1	E	1571	0	1499	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1571	0	1499	52	0
2	M	1840	0	1793	70	0
2	N	1840	0	1793	51	0
2	O	1840	0	1793	50	0
2	P	1840	0	1793	54	0
2	Q	1840	0	1793	69	0
2	R	1840	0	1793	69	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	1	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	3	0
4	R	4	0	5	1	0
5	M	24	0	10	8	0
5	N	24	0	10	10	0
5	O	24	0	10	9	0
5	P	24	0	10	8	0
5	Q	24	0	12	11	0
5	R	24	0	10	8	0
6	A	80	0	0	1	0
6	B	79	0	0	0	0
6	C	81	0	0	0	0
6	D	82	0	0	0	0
6	E	80	0	0	1	0
6	F	79	0	0	1	0
6	M	150	0	0	5	0
6	N	152	0	0	2	0
6	O	147	0	0	5	0
6	P	145	0	0	3	0
6	Q	149	0	0	6	0
6	R	150	0	0	3	0
All	All	22014	0	19844	596	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (596) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:491:ILE:HD11	5:N:550[A]:DHY:H72	1.23	1.20
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.26	1.16
1:E:165:GLN:H	1:E:165:GLN:NE2	1.50	1.10
1:B:165:GLN:H	1:B:165:GLN:HE21	1.05	1.04
1:E:165:GLN:HE21	1:E:165:GLN:N	1.55	1.03
2:Q:491:ILE:HD11	5:Q:550[A]:DHY:H72	1.42	0.99
2:P:491:ILE:HD11	5:P:550[A]:DHY:H72	1.43	0.99
2:O:462:HIS:CE1	5:O:550[B]:DHY:O4	2.15	0.96
2:M:491:ILE:HD11	5:M:550[A]:DHY:H72	1.47	0.96
1:B:165:GLN:H	1:B:165:GLN:NE2	1.64	0.94
2:R:491:ILE:HD11	5:R:550[A]:DHY:H72	1.48	0.93
2:N:462:HIS:CE1	5:N:550[B]:DHY:O4	2.21	0.92
2:R:497:ASN:ND2	2:R:499:GLU:H	1.67	0.90
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.03	0.89
2:N:449:TRP:CE3	5:N:550[B]:DHY:H72	2.07	0.88
2:R:497:ASN:HD22	2:R:499:GLU:H	1.20	0.88
1:D:165:GLN:H	1:D:165:GLN:HE21	1.21	0.87
2:Q:462:HIS:CE1	5:Q:550[B]:DHY:O4	2.27	0.87
2:O:491:ILE:HD11	5:O:550[A]:DHY:H72	1.55	0.87
1:E:98:THR:HB	1:E:100:ASP:OD1	1.74	0.86
2:R:361:HIS:H	2:R:361:HIS:CD2	1.93	0.86
2:Q:449:TRP:CE3	5:Q:550[A]:DHY:H71	2.11	0.86
2:Q:462:HIS:HE1	5:Q:550[B]:DHY:O4	1.58	0.85
2:R:449:TRP:CE3	5:R:550[A]:DHY:H71	2.11	0.85
1:C:64:ARG:NH1	1:C:100:ASP:O	2.10	0.85
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.92	0.84
2:N:491:ILE:CD1	5:N:550[A]:DHY:H72	2.06	0.84
1:F:64:ARG:NH1	1:F:100:ASP:O	2.11	0.84
2:M:497:ASN:ND2	2:M:499:GLU:H	1.75	0.83
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.60	0.83
2:M:497:ASN:HD22	2:M:499:GLU:H	1.26	0.82
2:Q:449:TRP:CE3	5:Q:550[B]:DHY:H72	2.15	0.82
2:O:462:HIS:HE1	5:O:550[B]:DHY:O4	1.56	0.81
2:R:462:HIS:CE1	5:R:550[B]:DHY:O4	2.32	0.81
2:R:361:HIS:H	2:R:361:HIS:HD2	1.29	0.81
1:D:64:ARG:NH1	1:D:100:ASP:O	2.14	0.80
2:Q:491:ILE:CD1	5:Q:550[A]:DHY:H72	2.12	0.80
1:A:67:PHE:CZ	1:A:94:ARG:HD3	2.17	0.80
2:M:449:TRP:CE3	5:M:550[B]:DHY:H72	2.17	0.80
2:M:462:HIS:CE1	5:M:550[B]:DHY:O4	2.35	0.80
2:R:449:TRP:CE3	5:R:550[B]:DHY:H72	2.17	0.80
2:O:449:TRP:CE3	5:O:550[B]:DHY:H72	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HB	1:A:100:ASP:OD1	1.84	0.78
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.63	0.78
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.48	0.78
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.47	0.78
1:A:67:PHE:HZ	1:A:94:ARG:HD3	1.49	0.78
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.83	0.77
2:R:536:GLU:HB2	6:R:1301:HOH:O	1.83	0.77
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.83	0.76
2:M:449:TRP:CE3	5:M:550[A]:DHY:H71	2.20	0.76
2:P:491:ILE:CD1	5:P:550[A]:DHY:H72	2.16	0.76
2:P:361:HIS:H	2:P:361:HIS:CD2	2.04	0.76
2:N:491:ILE:HD11	5:N:550[A]:DHY:C7	2.11	0.76
2:P:449:TRP:CE3	5:P:550[B]:DHY:H72	2.20	0.76
1:C:98:THR:HB	1:C:100:ASP:OD1	1.85	0.76
2:O:449:TRP:CE3	5:O:550[A]:DHY:H71	2.20	0.75
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.52	0.75
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.03	0.75
2:R:491:ILE:CD1	5:R:550[A]:DHY:H72	2.16	0.74
2:N:390:LYS:HE2	6:N:726:HOH:O	1.87	0.74
2:R:462:HIS:HE1	5:R:550[B]:DHY:O4	1.68	0.74
1:B:98:THR:HB	1:B:100:ASP:OD1	1.87	0.74
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.52	0.73
1:B:176:GLU:HG3	1:B:180:LYS:O	1.88	0.73
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.52	0.73
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.70	0.73
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.23	0.73
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.19	0.73
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.72	0.72
1:D:98:THR:HB	1:D:100:ASP:OD1	1.88	0.72
1:D:165:GLN:H	1:D:165:GLN:NE2	1.87	0.72
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.24	0.72
1:F:165:GLN:H	1:F:165:GLN:NE2	1.86	0.72
1:E:64:ARG:NH1	1:E:100:ASP:O	2.23	0.72
2:P:462:HIS:HE1	5:P:550[B]:DHY:O4	1.71	0.71
1:F:176:GLU:HG3	1:F:180:LYS:O	1.91	0.71
1:B:165:GLN:HE21	1:B:165:GLN:N	1.85	0.71
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.20	0.71
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.72	0.71
2:M:390:LYS:HD3	6:M:640:HOH:O	1.89	0.71
1:F:165:GLN:H	1:F:165:GLN:HE21	1.38	0.70
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:491:ILE:CD1	5:M:550[A]:DHY:H72	2.20	0.70
1:F:98:THR:HB	1:F:100:ASP:OD1	1.92	0.70
2:M:361:HIS:H	2:M:361:HIS:CD2	2.10	0.69
1:C:165:GLN:H	1:C:165:GLN:NE2	1.90	0.69
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.73	0.69
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.75	0.69
2:O:497:ASN:HD22	2:O:499:GLU:H	1.41	0.69
2:Q:390:LYS:HE2	6:Q:1109:HOH:O	1.93	0.68
2:R:497:ASN:HD22	2:R:497:ASN:C	2.00	0.68
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.75	0.68
2:P:361:HIS:H	2:P:361:HIS:HD2	1.41	0.68
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.43	0.68
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.29	0.67
2:Q:438:SER:O	4:Q:601:BME:H22	1.94	0.67
2:Q:462:HIS:CE1	5:Q:550[B]:DHY:HO4	2.11	0.67
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.43	0.67
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.95	0.67
2:P:449:TRP:CE3	5:P:550[A]:DHY:H71	2.30	0.67
1:A:176:GLU:HA	1:A:180:LYS:O	1.94	0.66
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.77	0.66
2:O:491:ILE:CD1	5:O:550[A]:DHY:H72	2.23	0.66
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.59	0.66
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.26	0.66
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.95	0.66
2:P:497:ASN:HD22	2:P:499:GLU:H	1.44	0.66
2:Q:536:GLU:HB2	6:Q:1072:HOH:O	1.94	0.66
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.30	0.66
1:B:78:GLU:HG2	2:N:301:PRO:CB	2.26	0.65
2:N:449:TRP:CE3	5:N:550[A]:DHY:H71	2.31	0.65
2:R:416:LEU:C	2:R:416:LEU:HD23	2.20	0.65
1:E:98:THR:O	1:E:102:GLY:HA2	1.97	0.65
1:D:100:ASP:CG	1:D:101:ALA:H	2.03	0.65
2:Q:390:LYS:HD3	6:Q:992:HOH:O	1.95	0.65
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.78	0.64
1:B:78:GLU:HG2	2:N:301:PRO:CG	2.27	0.64
2:N:361:HIS:CD2	2:N:361:HIS:H	2.14	0.64
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.78	0.64
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.63	0.64
2:P:376:GLU:OE1	6:P:639:HOH:O	2.15	0.64
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.95	0.64
2:R:405:GLY:HA3	6:R:1225:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.23	0.64
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.46	0.64
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.05	0.64
2:O:361:HIS:H	2:O:361:HIS:CD2	2.15	0.64
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.80	0.64
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.79	0.64
2:Q:405:GLY:HA3	6:Q:996:HOH:O	1.98	0.64
2:Q:449:TRP:CZ3	5:Q:550[A]:DHY:H71	2.33	0.63
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.81	0.63
1:C:176:GLU:OE2	1:C:179:GLY:HA2	1.98	0.63
1:B:176:GLU:HG3	1:B:180:LYS:C	2.24	0.63
2:Q:376:GLU:O	2:Q:442:ILE:HA	1.98	0.63
2:R:400:TRP:HA	2:R:425:GLY:O	1.99	0.63
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.80	0.63
2:P:405:GLY:HA3	6:P:647:HOH:O	1.99	0.62
1:E:176:GLU:HA	1:E:180:LYS:O	1.99	0.62
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.80	0.62
1:D:78:GLU:HG2	2:P:301:PRO:CB	2.29	0.62
2:O:497:ASN:ND2	2:O:499:GLU:H	1.96	0.62
2:P:376:GLU:O	2:P:442:ILE:HA	1.99	0.62
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.30	0.62
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.46	0.62
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	1.98	0.62
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.18	0.62
1:A:162:GLU:OE2	1:C:133:ARG:NH2	2.32	0.62
1:B:133:ARG:NH2	1:C:162:GLU:OE2	2.33	0.62
2:N:462:HIS:HE1	5:N:550[B]:DHY:O4	1.70	0.61
1:F:50:LEU:O	1:F:182:ALA:HA	1.99	0.61
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.83	0.61
1:F:78:GLU:HG2	2:R:301:PRO:CB	2.31	0.61
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.83	0.61
1:D:78:GLU:HG2	2:P:301:PRO:HB3	1.82	0.61
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.00	0.61
2:R:356:PHE:HD1	2:R:428:ARG:HD3	1.64	0.61
1:D:176:GLU:HG3	1:D:180:LYS:O	2.01	0.61
2:M:462:HIS:HE1	5:M:550[B]:DHY:O4	1.78	0.60
2:M:497:ASN:HD22	2:M:497:ASN:C	2.09	0.60
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.16	0.60
2:Q:306:SER:OG	2:Q:530:GLN:NE2	2.21	0.60
2:O:416:LEU:C	2:O:416:LEU:HD23	2.25	0.60
1:F:100:ASP:CG	1:F:101:ALA:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:371:GLY:HA3	2:Q:422:ASN:ND2	2.17	0.60
2:R:497:ASN:HD22	2:R:498:PRO:N	2.00	0.60
2:M:497:ASN:HD22	2:M:498:PRO:N	2.00	0.60
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.37	0.60
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.32	0.59
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.84	0.59
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.00	0.59
2:O:390:LYS:HD2	6:O:647:HOH:O	2.03	0.59
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.38	0.59
1:A:100:ASP:CG	1:A:101:ALA:H	2.11	0.59
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.17	0.59
1:C:78:GLU:HG2	2:O:301:PRO:HB3	1.84	0.58
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.36	0.58
2:O:376:GLU:O	2:O:442:ILE:HA	2.02	0.58
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.38	0.58
2:M:522:ARG:NH1	6:M:664:HOH:O	2.32	0.58
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.85	0.58
1:B:98:THR:O	1:B:102:GLY:HA2	2.04	0.58
2:M:478:LEU:HD23	2:M:478:LEU:C	2.28	0.58
1:F:19:ILE:O	2:R:426:VAL:HG21	2.03	0.58
2:Q:411:LYS:O	2:Q:414:ARG:NH1	2.37	0.58
2:Q:522:ARG:NH1	6:Q:1029:HOH:O	2.37	0.58
1:D:19:ILE:O	2:P:426:VAL:HG21	2.03	0.57
1:F:168:GLU:HA	1:F:171:ILE:HD13	1.85	0.57
2:R:416:LEU:HD23	2:R:417:ALA:N	2.18	0.57
2:M:413:ASP:C	2:M:414:ARG:HD2	2.29	0.57
2:N:449:TRP:CZ3	5:N:550[A]:DHY:H71	2.39	0.57
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.87	0.57
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.70	0.57
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.86	0.57
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.86	0.57
2:R:449:TRP:CZ3	5:R:550[A]:DHY:H71	2.39	0.57
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.86	0.57
2:N:497:ASN:HD22	2:N:499:GLU:H	1.53	0.57
2:O:403:ASN:HB2	6:O:612:HOH:O	2.03	0.57
2:M:361:HIS:H	2:M:361:HIS:HD2	1.49	0.57
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.87	0.57
2:M:416:LEU:C	2:M:416:LEU:HD23	2.30	0.56
1:D:132:ALA:HB3	1:D:135:ILE:HD12	1.86	0.56
2:Q:363:LEU:N	2:Q:363:LEU:HD12	2.20	0.56
2:M:449:TRP:CZ3	5:M:550[A]:DHY:H71	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:HG2	2:N:301:PRO:HB3	1.86	0.56
1:E:100:ASP:CG	1:E:101:ALA:H	2.12	0.56
1:F:131:PHE:O	1:F:132:ALA:HB2	2.04	0.56
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.88	0.56
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.85	0.56
1:C:131:PHE:O	1:C:132:ALA:HB2	2.05	0.56
2:M:390:LYS:HE2	6:M:717:HOH:O	2.05	0.56
1:C:78:GLU:HG2	2:O:301:PRO:CB	2.35	0.56
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.06	0.56
1:F:133:ARG:HG2	2:R:326:THR:HG21	1.87	0.56
2:R:497:ASN:HD22	2:R:499:GLU:N	1.97	0.56
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.41	0.56
2:P:413:ASP:O	2:P:414:ARG:NH1	2.39	0.56
2:Q:361:HIS:ND1	4:Q:601:BME:H21	2.20	0.56
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.53	0.56
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.88	0.56
2:P:416:LEU:C	2:P:416:LEU:HD23	2.31	0.56
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.36	0.56
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.21	0.55
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.06	0.55
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.03	0.55
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.95	0.55
1:F:32:ASP:HB2	6:F:1348:HOH:O	2.05	0.55
1:E:98:THR:OG1	1:E:102:GLY:N	2.39	0.55
1:C:98:THR:O	1:C:102:GLY:HA2	2.07	0.55
1:D:176:GLU:OE2	1:D:179:GLY:HA2	2.06	0.55
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.55
2:P:400:TRP:HA	2:P:425:GLY:O	2.06	0.55
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.32	0.55
1:A:114:VAL:HG23	1:A:122:MET:CE	2.37	0.54
2:N:361:HIS:H	2:N:361:HIS:HD2	1.55	0.54
1:D:98:THR:O	1:D:102:GLY:HA2	2.07	0.54
1:A:64:ARG:NH1	1:A:100:ASP:O	2.41	0.54
2:N:371:GLY:HA3	2:N:422:ASN:CG	2.33	0.54
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.89	0.54
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.90	0.54
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.90	0.54
2:P:478:LEU:C	2:P:478:LEU:HD23	2.33	0.54
2:Q:462:HIS:CE1	5:Q:550[A]:DHY:O3	2.61	0.54
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.43	0.54
1:D:18:HIS:CE1	1:D:99:PHE:CE1	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:451:ASN:HB3	2:R:455:ASP:OD2	2.07	0.54
2:P:484:PRO:O	2:P:488:MET:HE3	2.09	0.53
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.53
1:F:110:LYS:HE2	1:F:148:GLU:OE2	2.08	0.53
1:C:100:ASP:CG	1:C:101:ALA:H	2.16	0.53
1:C:165:GLN:H	1:C:165:GLN:HE21	1.52	0.53
2:O:413:ASP:O	2:O:414:ARG:NH1	2.41	0.53
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.23	0.53
1:D:15:PRO:HB3	1:D:133:ARG:HD2	1.89	0.53
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.53
2:Q:371:GLY:HA3	2:Q:422:ASN:CG	2.32	0.53
1:A:50:LEU:O	1:A:182:ALA:HA	2.08	0.53
2:P:307:ARG:CG	2:P:533:THR:HG22	2.36	0.53
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.73	0.53
1:D:114:VAL:HG23	1:D:122:MET:HE3	1.91	0.53
1:B:35:ILE:HG21	1:B:92:PHE:CE2	2.42	0.53
1:A:176:GLU:HG3	1:A:180:LYS:O	2.09	0.53
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.72	0.53
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.55	0.53
2:R:468:PRO:HD2	2:R:472:THR:HG21	1.91	0.53
2:N:400:TRP:HA	2:N:425:GLY:O	2.09	0.52
2:Q:453:PRO:CB	2:R:310:ILE:HD12	2.35	0.52
1:E:176:GLU:HG3	1:E:180:LYS:O	2.10	0.52
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.52
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.25	0.52
2:O:497:ASN:HD22	2:O:497:ASN:C	2.18	0.52
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.77	0.52
2:O:449:TRP:CZ3	5:O:550[A]:DHY:H71	2.44	0.52
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.91	0.52
2:M:399:MET:HA	2:M:462:HIS:O	2.10	0.52
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.10	0.52
1:A:165:GLN:CD	1:A:165:GLN:H	2.18	0.52
2:M:536:GLU:HB2	6:M:696:HOH:O	2.09	0.51
1:C:5:LEU:O	2:O:387:GLN:HG2	2.10	0.51
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.92	0.51
1:D:18:HIS:CE1	1:D:99:PHE:HE1	2.27	0.51
1:D:191:GLY:O	1:D:194:GLU:HB2	2.10	0.51
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.39	0.51
2:N:376:GLU:O	2:N:442:ILE:HA	2.10	0.51
1:C:44:ALA:O	1:C:48:HIS:NE2	2.29	0.51
2:R:359:HIS:O	2:R:366:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.42	0.51
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.33	0.51
1:F:180:LYS:HG2	1:F:181:THR:N	2.25	0.51
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.51
1:D:165:GLN:HE21	1:D:165:GLN:N	2.00	0.51
2:N:413:ASP:C	2:N:414:ARG:HD2	2.36	0.51
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.45	0.51
1:F:70:VAL:HG12	1:F:128:ILE:HG12	1.92	0.51
1:F:77:GLY:O	1:F:114:VAL:HG12	2.11	0.51
1:D:114:VAL:HG23	1:D:122:MET:CE	2.41	0.50
1:E:94:ARG:NH2	2:Q:398:GLU:OE2	2.44	0.50
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.27	0.50
1:C:41:LYS:NZ	1:C:86:GLU:O	2.44	0.50
2:R:399:MET:HA	2:R:462:HIS:O	2.11	0.50
2:N:478:LEU:C	2:N:478:LEU:HD23	2.35	0.50
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.47	0.50
1:C:176:GLU:HA	1:C:180:LYS:O	2.10	0.50
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.26	0.50
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.74	0.50
1:C:98:THR:OG1	1:C:102:GLY:N	2.44	0.50
2:N:536:GLU:HB2	6:N:704:HOH:O	2.12	0.50
2:M:328:ILE:HD12	2:N:335:ALA:HB2	1.94	0.50
2:N:413:ASP:O	2:N:414:ARG:NH1	2.44	0.50
2:O:413:ASP:C	2:O:414:ARG:HD2	2.37	0.50
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.93	0.50
2:O:359:HIS:O	2:O:366:ASN:HB3	2.12	0.50
1:E:133:ARG:HG2	2:Q:326:THR:HG21	1.93	0.50
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.56	0.50
2:R:413:ASP:C	2:R:414:ARG:HD2	2.37	0.50
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.27	0.49
1:B:143:LEU:C	1:B:143:LEU:HD23	2.37	0.49
2:P:522:ARG:NH1	6:P:666:HOH:O	2.44	0.49
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.47	0.49
2:Q:407:ARG:HD3	2:Q:417:ALA:O	2.12	0.49
2:R:478:LEU:C	2:R:478:LEU:HD23	2.37	0.49
1:B:52:LEU:C	1:B:52:LEU:HD22	2.38	0.49
2:N:306:SER:O	2:N:307:ARG:NH1	2.45	0.49
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.47	0.49
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.47	0.49
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.95	0.49
1:D:66:SER:HA	1:D:132:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:400:TRP:HA	2:O:425:GLY:O	2.11	0.49
2:R:522:ARG:HH21	2:R:524:ASP:CG	2.20	0.49
1:F:98:THR:OG1	1:F:102:GLY:N	2.41	0.49
2:R:306:SER:CB	2:R:530:GLN:HE21	2.25	0.49
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.94	0.48
2:Q:462:HIS:HE1	5:Q:550[A]:DHY:O3	1.95	0.48
2:Q:453:PRO:HB2	2:R:310:ILE:CD1	2.38	0.48
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.28	0.48
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.39	0.48
1:A:180:LYS:HG2	1:A:181:THR:N	2.28	0.48
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.49	0.48
1:D:176:GLU:HA	1:D:180:LYS:O	2.14	0.48
2:R:497:ASN:ND2	2:R:499:GLU:N	2.49	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.49	0.48
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.96	0.48
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.78	0.48
1:C:66:SER:HA	1:C:132:ALA:HB2	1.96	0.48
2:P:413:ASP:C	2:P:414:ARG:HD2	2.38	0.48
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.13	0.48
2:N:359:HIS:O	2:N:366:ASN:HB3	2.14	0.48
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.49	0.48
2:P:497:ASN:ND2	2:P:499:GLU:H	2.10	0.48
1:E:143:LEU:HD23	1:E:143:LEU:C	2.38	0.48
2:R:386:ASP:HA	2:R:527:LEU:O	2.13	0.48
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.96	0.47
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.61	0.47
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.79	0.47
2:P:489:CYS:HB3	2:P:492:VAL:HB	1.95	0.47
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.96	0.47
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.44	0.47
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.96	0.47
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.74	0.47
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.14	0.47
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.96	0.47
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.96	0.47
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.15	0.47
2:N:431:THR:HG22	2:N:437:TYR:HB3	1.97	0.47
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.80	0.47
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.15	0.47
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.82	0.47
1:A:67:PHE:CE1	1:A:94:ARG:HD3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:O	1:B:182:ALA:HA	2.14	0.47
1:B:94:ARG:NH2	2:N:398:GLU:OE2	2.46	0.47
2:N:488:MET:HE2	1:C:1:PRO:HG2	1.97	0.47
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.97	0.47
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.97	0.47
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.15	0.47
2:M:416:LEU:C	2:M:416:LEU:CD2	2.88	0.47
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.50	0.47
2:O:324:TYR:OH	5:O:550[A]:DHY:O1	2.28	0.47
1:D:143:LEU:C	1:D:143:LEU:HD23	2.40	0.47
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.47	0.47
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.50	0.47
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.97	0.47
1:E:165:GLN:H	1:E:165:GLN:HE21	0.69	0.47
1:E:78:GLU:HG2	2:Q:301:PRO:HB3	1.97	0.47
2:N:497:ASN:ND2	2:N:499:GLU:H	2.13	0.47
1:C:19:ILE:O	2:O:426:VAL:HG21	2.15	0.47
1:A:64:ARG:NE	6:A:219:HOH:O	2.44	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.46
2:O:486:ILE:N	2:O:487:PRO:HD2	2.30	0.46
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.96	0.46
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.82	0.46
2:O:356:PHE:CD1	2:O:428:ARG:CD	2.98	0.46
1:D:131:PHE:O	1:D:132:ALA:HB2	2.14	0.46
2:R:437:TYR:CD1	2:R:437:TYR:C	2.93	0.46
1:D:51:LEU:O	1:D:105:THR:HA	2.14	0.46
2:N:516:MET:HE3	2:N:516:MET:HB3	1.74	0.46
2:O:361:HIS:HD2	6:O:704:HOH:O	1.98	0.46
1:E:165:GLN:NE2	1:E:165:GLN:N	2.34	0.46
2:Q:399:MET:HA	2:Q:462:HIS:O	2.15	0.46
2:P:324:TYR:OH	5:P:550[A]:DHY:O1	2.23	0.46
2:P:449:TRP:CZ3	5:P:550[A]:DHY:H71	2.51	0.46
1:E:131:PHE:O	1:E:132:ALA:HB2	2.16	0.46
1:B:100:ASP:CG	1:B:101:ALA:H	2.24	0.46
2:N:399:MET:HA	2:N:462:HIS:O	2.16	0.46
2:M:414:ARG:HD2	2:M:414:ARG:N	2.31	0.46
2:N:373:PRO:HB3	2:N:423:PHE:HB2	1.98	0.46
1:C:36:TRP:CG	1:C:37:ASN:H	2.34	0.46
1:C:100:ASP:OD1	1:C:100:ASP:N	2.35	0.46
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.33	0.46
1:E:161:ILE:HD13	1:E:196:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:CG	2:O:301:PRO:HG3	2.46	0.45
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.28	0.45
1:D:100:ASP:CG	1:D:101:ALA:N	2.73	0.45
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.97	0.45
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.98	0.45
1:F:176:GLU:HG3	1:F:180:LYS:C	2.40	0.45
2:N:371:GLY:HA3	2:N:422:ASN:ND2	2.31	0.45
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.14	0.45
2:P:431:THR:HG22	2:P:437:TYR:HB3	1.98	0.45
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.82	0.45
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.46	0.45
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.16	0.45
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.31	0.45
1:F:114:VAL:HG23	1:F:122:MET:CE	2.46	0.45
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.97	0.45
2:R:376:GLU:O	2:R:442:ILE:HA	2.17	0.45
2:M:362:ASP:OD2	2:M:440:ARG:NH1	2.50	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.76	0.45
1:E:180:LYS:CG	1:E:181:THR:N	2.80	0.45
2:Q:390:LYS:CD	6:Q:992:HOH:O	2.59	0.45
2:Q:522:ARG:HH11	2:Q:522:ARG:HD3	1.55	0.45
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.16	0.45
2:M:354:LEU:HD23	2:M:356:PHE:CE1	2.52	0.45
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.97	0.45
2:N:449:TRP:CE3	5:N:550[B]:DHY:C7	2.89	0.45
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.80	0.45
1:B:64:ARG:NH1	1:B:100:ASP:O	2.50	0.45
1:D:98:THR:OG1	1:D:102:GLY:N	2.46	0.45
2:R:522:ARG:NH1	6:R:1258:HOH:O	2.48	0.45
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.44	0.44
1:D:36:TRP:CG	1:D:37:ASN:H	2.34	0.44
2:R:361:HIS:CD2	2:R:361:HIS:N	2.65	0.44
2:M:497:ASN:ND2	2:M:499:GLU:N	2.54	0.44
1:C:50:LEU:O	1:C:182:ALA:HA	2.17	0.44
1:D:67:PHE:HZ	1:D:94:ARG:CD	2.27	0.44
2:Q:449:TRP:CD2	5:Q:550[B]:DHY:H72	2.51	0.44
1:A:92:PHE:CG	2:M:349:PRO:HG3	2.53	0.44
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.74	0.44
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.52	0.44
2:M:448:PRO:HB2	2:P:516:MET:HA	1.98	0.44
1:C:19:ILE:CD1	2:O:408:TYR:HD2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.17	0.44
1:E:116:ASN:C	1:E:116:ASN:OD1	2.59	0.44
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.52	0.44
1:F:120:VAL:HA	1:F:121:PRO:HD3	1.84	0.44
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.73	0.44
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.80	0.44
1:F:110:LYS:CE	1:F:148:GLU:OE2	2.66	0.44
1:B:180:LYS:HG2	1:B:181:THR:N	2.33	0.44
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.53	0.43
2:M:488:MET:HE1	2:P:508:LEU:HD23	1.99	0.43
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.17	0.43
2:O:361:HIS:CD2	6:O:704:HOH:O	2.71	0.43
2:O:478:LEU:HD23	2:O:478:LEU:C	2.43	0.43
2:O:497:ASN:HD22	2:O:498:PRO:N	2.15	0.43
2:R:411:LYS:O	2:R:414:ARG:NH1	2.50	0.43
2:M:405:GLY:HA3	6:M:643:HOH:O	2.17	0.43
2:O:361:HIS:CG	4:O:601:BME:H21	2.53	0.43
1:E:133:ARG:HD3	1:E:133:ARG:HH11	1.62	0.43
1:F:143:LEU:C	1:F:143:LEU:HD23	2.43	0.43
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.88	0.43
2:R:449:TRP:CD2	5:R:550[B]:DHY:H72	2.52	0.43
1:B:70:VAL:HG21	1:B:106:LEU:HD21	2.00	0.43
2:R:431:THR:HG22	2:R:437:TYR:HB3	2.00	0.43
2:M:446:PRO:HD2	2:P:376:GLU:HG2	2.00	0.43
1:B:140:HIS:O	1:B:197:PHE:HA	2.18	0.43
1:C:52:LEU:C	1:C:52:LEU:HD22	2.44	0.43
2:P:362:ASP:OD2	2:P:440:ARG:NH1	2.52	0.43
1:E:180:LYS:HG2	1:E:181:THR:N	2.34	0.43
1:A:165:GLN:NE2	1:A:165:GLN:H	2.16	0.43
2:M:449:TRP:CD2	5:M:550[B]:DHY:H72	2.52	0.43
1:B:8:THR:HA	1:B:9:PRO:HD3	1.90	0.43
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.53	0.43
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.99	0.43
1:E:6:PRO:HG2	2:Q:503:GLN:NE2	2.33	0.43
1:A:35:ILE:CD1	2:M:351:PHE:CE1	3.02	0.43
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.54	0.43
2:M:361:HIS:CG	4:M:601:BME:H21	2.53	0.43
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.99	0.43
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.33	0.43
1:F:4:LEU:HB3	2:R:387:GLN:HB3	2.00	0.43
1:F:36:TRP:CG	1:F:37:ASN:H	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.00	0.43
1:C:63:VAL:HG12	1:C:66:SER:HB3	2.00	0.43
1:E:188:ARG:HH11	1:E:188:ARG:CG	2.32	0.43
2:Q:383:ARG:N	2:Q:524:ASP:OD1	2.47	0.43
1:F:19:ILE:O	2:R:426:VAL:CG2	2.65	0.43
2:O:390:LYS:CD	6:O:647:HOH:O	2.65	0.42
1:D:78:GLU:HG2	2:P:301:PRO:HG3	2.00	0.42
1:C:110:LYS:NZ	1:C:147:ASP:OD1	2.52	0.42
1:E:36:TRP:CG	1:E:37:ASN:H	2.37	0.42
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.18	0.42
1:A:4:LEU:HB3	2:M:387:GLN:HB3	2.02	0.42
1:A:8:THR:HA	1:A:9:PRO:HD3	1.88	0.42
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.45	0.42
2:N:486:ILE:HB	2:N:487:PRO:HD3	2.00	0.42
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.00	0.42
1:C:143:LEU:HD23	1:C:143:LEU:C	2.45	0.42
2:O:437:TYR:CD1	2:O:437:TYR:C	2.96	0.42
1:D:19:ILE:HD13	1:D:19:ILE:HG21	1.62	0.42
2:R:473:LYS:HD2	2:R:474:LEU:N	2.34	0.42
1:D:50:LEU:O	1:D:182:ALA:HA	2.19	0.42
2:P:326:THR:HG22	2:P:330:ARG:HD2	2.01	0.42
1:F:8:THR:HA	1:F:9:PRO:HD3	1.85	0.42
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.44	0.42
1:A:52:LEU:C	1:A:52:LEU:HD22	2.44	0.42
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.89	0.42
1:E:70:VAL:HG12	1:E:128:ILE:HG12	2.02	0.42
6:E:242:HOH:O	2:Q:426:VAL:HG21	2.18	0.42
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.42
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.83	0.42
1:A:98:THR:O	1:A:102:GLY:HA2	2.19	0.42
1:D:19:ILE:HG22	1:D:26:ALA:HB1	2.02	0.42
1:E:41:LYS:O	1:E:44:ALA:N	2.48	0.42
2:M:335:ALA:HB2	2:O:328:ILE:HD12	2.01	0.42
2:M:409:ARG:NH2	2:M:420:ASP:O	2.53	0.42
1:B:70:VAL:HA	1:B:127:ASN:O	2.19	0.42
2:O:395:THR:O	2:O:430:LEU:HA	2.19	0.42
2:P:449:TRP:CD2	5:P:550[B]:DHY:H72	2.54	0.42
1:E:41:LYS:HZ1	1:E:86:GLU:HA	1.85	0.42
2:Q:522:ARG:NE	2:Q:524:ASP:OD1	2.52	0.42
2:M:411:LYS:O	2:M:414:ARG:NH1	2.52	0.42
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:363:LEU:N	2:M:363:LEU:HD12	2.35	0.42
1:E:50:LEU:O	1:E:182:ALA:HA	2.20	0.42
1:F:37:ASN:HB2	1:F:106:LEU:HD12	2.01	0.42
1:F:51:LEU:HD23	1:F:183:TYR:HB2	2.02	0.42
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.19	0.42
2:R:383:ARG:HA	2:R:435:GLY:O	2.20	0.42
1:A:176:GLU:HG3	1:A:180:LYS:N	2.35	0.42
2:M:356:PHE:HD1	2:M:428:ARG:CD	2.26	0.42
2:M:400:TRP:HA	2:M:425:GLY:O	2.19	0.42
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.91	0.42
1:C:116:ASN:OD1	1:C:116:ASN:C	2.62	0.42
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.50	0.42
2:P:416:LEU:C	2:P:416:LEU:CD2	2.93	0.42
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.54	0.42
2:R:304:ASP:HB2	2:R:343:ILE:HB	2.02	0.42
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.35	0.41
2:O:381:ALA:O	2:O:522:ARG:HA	2.20	0.41
2:P:516:MET:HE3	2:P:516:MET:HB3	1.81	0.41
1:E:22:ALA:O	1:E:25:ALA:HB3	2.19	0.41
1:F:5:LEU:O	2:R:387:GLN:HG2	2.19	0.41
2:Q:395:THR:O	2:Q:430:LEU:HA	2.21	0.41
1:F:167:ARG:O	1:F:171:ILE:HD12	2.20	0.41
2:R:316:HIS:HB3	2:R:317:PRO:HD2	2.02	0.41
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.03	0.41
1:A:36:TRP:CG	1:A:37:ASN:H	2.38	0.41
1:F:35:ILE:HD13	2:R:351:PHE:CE1	2.55	0.41
2:N:416:LEU:HD23	2:N:416:LEU:C	2.45	0.41
1:D:58:GLY:HA3	1:D:190:GLN:OE1	2.20	0.41
1:A:63:VAL:HG13	2:M:330:ARG:CZ	2.50	0.41
1:B:52:LEU:HA	1:B:104:TRP:O	2.21	0.41
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.54	0.41
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.67	0.41
1:A:54:GLN:HG2	1:A:102:GLY:O	2.20	0.41
2:M:359:HIS:O	2:M:366:ASN:HB3	2.21	0.41
2:M:376:GLU:HG2	2:P:446:PRO:HD2	2.03	0.41
1:C:176:GLU:HG3	1:C:180:LYS:C	2.45	0.41
1:C:180:LYS:HG2	1:C:181:THR:N	2.35	0.41
1:D:8:THR:HA	1:D:9:PRO:HD3	1.89	0.41
2:Q:416:LEU:C	2:Q:416:LEU:CD2	2.93	0.41
2:R:361:HIS:ND1	4:R:601:BME:H21	2.35	0.41
2:M:510:MET:HE1	2:P:456:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:SER:HA	1:F:132:ALA:HB2	2.03	0.41
1:F:70:VAL:HA	1:F:127:ASN:O	2.21	0.41
1:F:174:ARG:HE	1:F:181:THR:HG23	1.84	0.41
1:B:176:GLU:HA	1:B:180:LYS:O	2.20	0.40
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.83	0.40
2:P:411:LYS:O	2:P:414:ARG:NH1	2.53	0.40
1:E:58:GLY:HA3	1:E:190:GLN:OE1	2.21	0.40
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.21	0.40
2:Q:451:ASN:HB3	2:Q:452:GLY:H	1.69	0.40
1:F:70:VAL:HG21	1:F:106:LEU:HD21	2.02	0.40
2:R:414:ARG:HD2	2:R:414:ARG:N	2.36	0.40
2:M:484:PRO:O	2:M:488:MET:HE3	2.21	0.40
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.57	0.40
2:N:432:ASP:OD1	2:N:432:ASP:C	2.63	0.40
2:N:449:TRP:CD2	5:N:550[B]:DHY:H72	2.51	0.40
1:C:140:HIS:O	1:C:197:PHE:HA	2.22	0.40
1:D:33:GLN:OE1	2:P:355:GLY:N	2.39	0.40
1:F:78:GLU:HG2	2:R:301:PRO:HB3	2.02	0.40
2:N:495:ILE:HG21	2:N:500:ALA:HB3	2.04	0.40
1:C:51:LEU:O	1:C:105:THR:HA	2.21	0.40
2:O:449:TRP:CD2	5:O:550[B]:DHY:H72	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	D	198/200 (99%)	190 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	F	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
2	M	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
All	All	2562/2628 (98%)	2469 (96%)	93 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	155 (96%)	7 (4%)	26	44
1	B	162/163 (99%)	153 (94%)	9 (6%)	19	33
1	C	162/163 (99%)	153 (94%)	9 (6%)	19	33
1	D	162/163 (99%)	157 (97%)	5 (3%)	35	57
1	E	162/163 (99%)	155 (96%)	7 (4%)	26	44
1	F	162/163 (99%)	155 (96%)	7 (4%)	26	44
2	M	196/202 (97%)	185 (94%)	11 (6%)	19	33
2	N	196/202 (97%)	188 (96%)	8 (4%)	27	46
2	O	196/202 (97%)	191 (97%)	5 (3%)	40	63
2	P	196/202 (97%)	185 (94%)	11 (6%)	19	33
2	Q	196/202 (97%)	189 (96%)	7 (4%)	31	52
2	R	196/202 (97%)	188 (96%)	8 (4%)	27	46
All	All	2148/2190 (98%)	2054 (96%)	94 (4%)	25	43

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	52	LEU
1	A	106	LEU
1	A	143	LEU
1	A	165	GLN
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	428	ARG
2	M	433	SER
2	M	434	ASP
2	M	478	LEU
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	52	LEU
1	B	106	LEU
1	B	128	ILE
1	B	143	LEU
1	B	158	LEU
1	B	165	GLN
2	N	364	LEU
2	N	395	THR
2	N	416	LEU
2	N	428	ARG
2	N	442	ILE
2	N	478	LEU
2	N	499	GLU
2	N	507	LYS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	78	GLU
1	C	94	ARG
1	C	133	ARG

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Mol	Chain	Res	Type
1	C	165	GLN
1	C	181	THR
2	O	393	PRO
2	O	395	THR
2	O	416	LEU
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	52	LEU
1	D	154	LYS
1	D	165	GLN
2	P	364	LEU
2	P	395	THR
2	P	416	LEU
2	P	428	ARG
2	P	434	ASP
2	P	440	ARG
2	P	478	LEU
2	P	497	ASN
2	P	499	GLU
2	P	511	ASN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	32	ASP
1	E	52	LEU
1	E	94	ARG
1	E	165	GLN
1	E	188	ARG
2	Q	364	LEU
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	478	LEU
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	66	SER
1	F	78	GLU

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Mol	Chain	Res	Type
1	F	94	ARG
1	F	165	GLN
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP
2	R	442	ILE
2	R	478	LEU
2	R	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	59	ASN
1	A	163	GLN
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	11	GLN
1	B	140	HIS
1	B	163	GLN
1	B	165	GLN
2	N	334	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	163	GLN
1	C	165	GLN
2	O	305	ASN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	163	GLN
1	D	165	GLN

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Mol	Chain	Res	Type
2	P	334	GLN
2	P	359	HIS
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	163	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	59	ASN
1	F	76	ASN
1	F	163	GLN
1	F	165	GLN
2	R	359	HIS
2	R	361	HIS
2	R	394	ASN
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	DHY	O	550[A]	3	12,12,12	2.00	4 (33%)	16,16,16	1.80	5 (31%)
4	BME	Q	601	2	3,3,3	0.49	0	2,2,2	0.54	0
5	DHY	P	550[A]	3	12,12,12	1.92	3 (25%)	16,16,16	1.64	3 (18%)
5	DHY	M	550[B]	3	12,12,12	1.82	3 (25%)	16,16,16	2.59	7 (43%)
5	DHY	Q	550[B]	3	12,12,12	1.67	3 (25%)	16,16,16	2.37	7 (43%)
5	DHY	O	550[B]	3	12,12,12	1.83	3 (25%)	16,16,16	2.64	8 (50%)
5	DHY	P	550[B]	3	12,12,12	1.85	3 (25%)	16,16,16	2.43	6 (37%)
5	DHY	M	550[A]	3	12,12,12	2.12	5 (41%)	16,16,16	1.81	3 (18%)
5	DHY	R	550[A]	3	12,12,12	1.91	5 (41%)	16,16,16	1.73	3 (18%)
4	BME	R	601	2	3,3,3	0.31	0	2,2,2	0.51	0
4	BME	N	601	2	3,3,3	0.15	0	2,2,2	0.03	0
4	BME	M	601	2	3,3,3	0.31	0	2,2,2	0.52	0
5	DHY	N	550[A]	3	12,12,12	1.79	3 (25%)	16,16,16	1.90	5 (31%)
5	DHY	R	550[B]	3	12,12,12	1.67	2 (16%)	16,16,16	2.47	7 (43%)
4	BME	O	601	2	3,3,3	0.39	0	2,2,2	0.30	0
5	DHY	N	550[B]	3	12,12,12	1.87	4 (33%)	16,16,16	2.69	9 (56%)
5	DHY	Q	550[A]	3	12,12,12	1.85	5 (41%)	16,16,16	1.52	3 (18%)
4	BME	P	601	2	3,3,3	0.49	0	2,2,2	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DHY	O	550[A]	3	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	-
5	DHY	P	550[A]	3	-	0/4/4/4	0/1/1/1
5	DHY	M	550[B]	3	-	0/4/4/4	0/1/1/1
5	DHY	Q	550[B]	3	-	0/4/4/4	0/1/1/1
5	DHY	O	550[B]	3	-	0/4/4/4	0/1/1/1
5	DHY	P	550[B]	3	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DHY	M	550[A]	3	-	0/4/4/4	0/1/1/1
5	DHY	R	550[A]	3	-	0/4/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	-
4	BME	N	601	2	-	0/1/1/1	-
4	BME	M	601	2	-	1/1/1/1	-
5	DHY	N	550[A]	3	-	0/4/4/4	0/1/1/1
5	DHY	R	550[B]	3	-	0/4/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	-
5	DHY	N	550[B]	3	-	0/4/4/4	0/1/1/1
5	DHY	Q	550[A]	3	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550[A]	DHY	C7-C8	4.56	1.60	1.51
5	N	550[B]	DHY	C7-C8	4.36	1.60	1.51
5	M	550[B]	DHY	C7-C8	4.22	1.60	1.51
5	P	550[A]	DHY	C7-C8	4.18	1.60	1.51
5	P	550[B]	DHY	C7-C8	3.89	1.59	1.51
5	O	550[B]	DHY	C7-C8	3.71	1.59	1.51
5	Q	550[B]	DHY	C7-C8	3.64	1.58	1.51
5	R	550[B]	DHY	C7-C8	3.60	1.58	1.51
5	R	550[A]	DHY	C7-C8	3.59	1.58	1.51
5	O	550[A]	DHY	C7-C8	3.47	1.58	1.51
5	Q	550[A]	DHY	C7-C8	3.27	1.58	1.51
5	N	550[A]	DHY	C7-C8	3.26	1.58	1.51
5	N	550[A]	DHY	C7-C1	3.24	1.56	1.51
5	M	550[A]	DHY	C7-C1	3.18	1.56	1.51
5	P	550[A]	DHY	C7-C1	3.10	1.56	1.51
5	Q	550[A]	DHY	C7-C1	2.96	1.56	1.51
5	R	550[B]	DHY	C6-C1	2.95	1.44	1.38
5	O	550[A]	DHY	C2-C1	2.91	1.44	1.39
5	O	550[A]	DHY	C7-C1	2.89	1.56	1.51
5	Q	550[B]	DHY	C6-C1	2.76	1.44	1.38
5	O	550[B]	DHY	C6-C1	2.67	1.44	1.38
5	M	550[B]	DHY	C6-C1	2.65	1.44	1.38
5	O	550[B]	DHY	C6-C5	2.59	1.43	1.38
5	N	550[B]	DHY	C6-C1	2.58	1.44	1.38
5	R	550[A]	DHY	C2-C1	2.56	1.43	1.39
5	M	550[A]	DHY	C2-C1	2.55	1.43	1.39
5	O	550[A]	DHY	O2-C8	-2.54	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	550[A]	DHY	C6-C5	2.45	1.42	1.38
5	P	550[B]	DHY	C7-C1	2.38	1.55	1.51
5	P	550[B]	DHY	C6-C1	2.33	1.43	1.38
5	M	550[A]	DHY	O2-C8	-2.32	1.23	1.30
5	M	550[B]	DHY	C6-C5	2.32	1.42	1.38
5	R	550[A]	DHY	C7-C1	2.31	1.55	1.51
5	N	550[B]	DHY	C7-C1	2.29	1.55	1.51
5	Q	550[A]	DHY	O2-C8	-2.27	1.23	1.30
5	M	550[A]	DHY	C6-C5	2.21	1.42	1.38
5	N	550[A]	DHY	C2-C1	2.19	1.43	1.39
5	Q	550[A]	DHY	O1-C8	2.18	1.29	1.22
5	Q	550[B]	DHY	C7-C1	2.16	1.55	1.51
5	N	550[B]	DHY	C6-C5	2.15	1.42	1.38
5	R	550[A]	DHY	O2-C8	-2.10	1.23	1.30
5	P	550[A]	DHY	O2-C8	-2.07	1.24	1.30
5	Q	550[A]	DHY	C2-C1	2.05	1.42	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	550[B]	DHY	O1-C8-C7	-5.67	105.85	122.94
5	O	550[B]	DHY	O1-C8-C7	-5.56	106.16	122.94
5	N	550[B]	DHY	O1-C8-C7	-5.31	106.91	122.94
5	R	550[B]	DHY	O1-C8-C7	-5.13	107.47	122.94
5	P	550[B]	DHY	O1-C8-C7	-5.09	107.60	122.94
5	Q	550[B]	DHY	C7-C1-C6	-4.93	113.64	120.89
5	N	550[B]	DHY	C7-C1-C6	-4.76	113.89	120.89
5	M	550[B]	DHY	C7-C1-C6	-4.52	114.25	120.89
5	O	550[B]	DHY	C7-C1-C6	-4.45	114.34	120.89
5	Q	550[B]	DHY	O1-C8-C7	-4.40	109.67	122.94
5	R	550[B]	DHY	C7-C1-C6	-4.37	114.46	120.89
5	P	550[B]	DHY	C7-C1-C6	-4.36	114.48	120.89
5	N	550[B]	DHY	C6-C5-C4	-3.74	116.76	120.50
5	Q	550[B]	DHY	C7-C1-C2	3.66	125.94	120.38
5	N	550[A]	DHY	C3-C2-C1	-3.64	117.03	120.81
5	M	550[B]	DHY	C5-C4-C3	3.37	123.25	119.66
5	R	550[B]	DHY	C7-C1-C2	3.33	125.44	120.38
5	O	550[A]	DHY	O1-C8-C7	-3.32	112.92	122.94
5	O	550[B]	DHY	C6-C5-C4	-3.32	117.18	120.50
5	M	550[A]	DHY	C3-C2-C1	-3.32	117.36	120.81
5	O	550[B]	DHY	O2-C8-C7	3.30	126.56	113.98
5	N	550[B]	DHY	C7-C1-C2	3.25	125.32	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	550[B]	DHY	C5-C4-C3	3.24	123.11	119.66
5	P	550[A]	DHY	O1-C8-C7	-3.23	113.21	122.94
5	M	550[B]	DHY	C7-C1-C2	3.21	125.25	120.38
5	M	550[B]	DHY	C6-C5-C4	-3.21	117.29	120.50
5	R	550[B]	DHY	C5-C4-C3	3.20	123.07	119.66
5	P	550[B]	DHY	C7-C1-C2	3.17	125.20	120.38
5	R	550[B]	DHY	O2-C8-C7	3.13	125.93	113.98
5	M	550[A]	DHY	O1-C8-C7	-3.05	113.73	122.94
5	Q	550[B]	DHY	O2-C8-C7	2.99	125.37	113.98
5	M	550[B]	DHY	O2-C8-C7	2.99	125.37	113.98
5	O	550[A]	DHY	C3-C2-C1	-2.95	117.75	120.81
5	Q	550[A]	DHY	O1-C8-C7	-2.94	114.08	122.94
5	N	550[B]	DHY	C5-C4-C3	2.91	122.77	119.66
5	O	550[B]	DHY	C7-C1-C2	2.88	124.76	120.38
5	P	550[B]	DHY	O2-C8-C7	2.85	124.84	113.98
5	R	550[A]	DHY	O1-C8-C7	-2.85	114.36	122.94
5	R	550[A]	DHY	C3-C2-C1	-2.83	117.87	120.81
5	M	550[A]	DHY	C2-C3-C4	2.80	122.47	119.89
5	P	550[B]	DHY	C6-C5-C4	-2.78	117.71	120.50
5	R	550[B]	DHY	C6-C5-C4	-2.77	117.72	120.50
5	R	550[A]	DHY	C2-C3-C4	2.70	122.38	119.89
5	N	550[A]	DHY	O1-C8-C7	-2.67	114.90	122.94
5	O	550[A]	DHY	O2-C8-C7	2.62	123.96	113.98
5	P	550[A]	DHY	C3-C2-C1	-2.61	118.11	120.81
5	P	550[B]	DHY	C5-C4-C3	2.59	122.42	119.66
5	N	550[B]	DHY	O2-C8-O1	2.58	129.96	123.33
5	Q	550[A]	DHY	C3-C2-C1	-2.53	118.19	120.81
5	Q	550[B]	DHY	C6-C5-C4	-2.52	117.98	120.50
5	N	550[A]	DHY	C2-C3-C4	2.41	122.11	119.89
5	N	550[B]	DHY	O2-C8-C7	2.34	122.92	113.98
5	N	550[B]	DHY	C3-C2-C1	-2.30	118.43	120.81
5	P	550[A]	DHY	C2-C3-C4	2.29	122.00	119.89
5	Q	550[B]	DHY	C5-C4-C3	2.27	122.09	119.66
5	O	550[B]	DHY	C3-C2-C1	-2.25	118.48	120.81
5	N	550[B]	DHY	O3-C3-C2	2.20	125.39	119.45
5	Q	550[B]	DHY	C3-C2-C1	-2.16	118.57	120.81
5	R	550[B]	DHY	C3-C2-C1	-2.16	118.57	120.81
5	N	550[A]	DHY	C7-C1-C6	-2.15	117.73	120.89
5	O	550[A]	DHY	C2-C3-C4	2.12	121.84	119.89
5	Q	550[A]	DHY	C2-C3-C4	2.11	121.83	119.89
5	M	550[B]	DHY	O2-C8-O1	2.07	128.65	123.33
5	O	550[A]	DHY	O4-C4-C5	2.06	124.88	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550[A]	DHY	O4-C4-C5	2.05	124.87	119.36
5	O	550[B]	DHY	O3-C3-C2	2.03	124.94	119.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	601	BME	O1-C1-C2-S2

There are no ring outliers.

16 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	550[A]	DHY	5	0
4	Q	601	BME	3	0
5	P	550[A]	DHY	5	0
5	M	550[B]	DHY	4	0
5	Q	550[B]	DHY	5	0
5	O	550[B]	DHY	4	0
5	P	550[B]	DHY	3	0
5	M	550[A]	DHY	4	0
5	R	550[A]	DHY	4	0
4	R	601	BME	1	0
4	M	601	BME	1	0
5	N	550[A]	DHY	5	0
5	R	550[B]	DHY	4	0
4	O	601	BME	1	0
5	N	550[B]	DHY	5	0
5	Q	550[A]	DHY	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.